201-15693

NCIC OPPT/DC/USEPA/US
Sent by: JuanB Perez

11/09/2004 03:09 PM

To NCIC HPV@EPA
cc
bcc
Subject Re: FW: HPV Submission

--
US Environmental Protection Agency
Office of Pollution Prevention and Toxics Docket
Non-Confidential Information Center (MC 7407T)
(operated by ASRC Aerospace Corporation)
1301 Constitution Ave NW Room B146 EPA West
Washington DC 20460
phone 202-566-0280 * fax 202-566-0282 * e-mail oppt.ncic@epa.gov
"Hartwell, Gail" <ggarvin@dow.com>

"Hartwell, Gail"
<ggarvin@dow.com>
11/09/2004 01:47 PM

To NCIC OPPT@EPA, Rtk Chem@EPA
cc
Subject FW: HPV Submission

EPA,
After reviewing the HPV database, I realized that the data for 2,4-dichlorophenol sodium salt has never been posted. This information was sent to your organization in August 2003.

Let me know if you have any questions,
Gail M. Hartwell
EH&S Delivery Specialist
Dow AgroSciences LLC
9330 Zionsville Road
Indianapolis, IN 46268
(317) 337-3609
ggarvin@dow.com

> -----Original Message-----
> From: Berdasco, Nancy (NM)
> Sent: Wednesday, August 27, 2003 10:26 AM
> To: 'chem.rtk@epa.gov'
> Cc: Burgert, Linda (LC); Clark, Martin (JT); Garvin, Gail
> Subject: FW: HPV Submission
>
> Sir: Enclosed is an additional HPV document which is supplemental to the posting referenced in the e-mail below of 8/11/03. Since the test plan 2,4-dichlorophenol sodium salt (CAS # 3757-76-4) indicates that, in the mammalian body, the chemical is present as 2,4-dichlorophenol (CAS # 120-83-2), we are including robust summaries for mammalian endpoints for 2,4-dichlorophenol. The document below is a SIDS dossier for 2,4-dichlorophenol (CAS # 120-83-2). Please include it in the posting of HPV documents for 2,4-dichlorophenol sodium salt (CAS # 3757-76-4).
>
> > <<120832_SIAR.PDF>>
>
> Nancy
> Nancy Anne M. Berdasco
> EH&S Product Regulatory Management
> 1803 Building
> 6-0245
>
> -----Original Message-----
> From: Berdasco, Nancy (NM)
> Sent: Monday, August 11, 2003 1:39 PM
> To: 'chem.rtk@epa.gov'
> Cc: Burgert, Linda (LC); Clark, Martin (JT); Garvin, Gail
> Subject: HPV Submission
>
> Sir: Enclosed are the HPV documents for 2,4-dichlorophenol sodium salt (CAS # 3757-76-4) which we wish to have posted on the EPA website for HPV chemicals. For the chemical, there is a cover letter, test plan and the IUCLID document. This information has been added to the US HPV Chemical Tracking System at http://www.hpvchallenge.com <http://www.hpvchallenge.com> . Please let us know if you have any questions.
> > <<dichlorophenol3757764EPAletter.pdf>>

>
> > <<24DCPNa.PDF>> > > <<Plan.PDF>>
>
> Nancy
> Nancy Anne M. Berdasco
> EH&S Product Regulatory Management
> 1803 Building
> 6-0245
>


120832_SIAR.PDF

dichlorophenol3757764EPAletter.pdf

24DCPNa.PDF

Plan.PDF

201-15693

Dow AgroSciences LLC
9330 Zionsville Road
Indianapolis, IN 46268

Dow AgroSciences

Ms. Marianne L. Horinko
Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

August 6, 2003

Dear Ms. Horinko:

CHEMICAL RIGHT TO KNOW – HPV CHALLENGE PROGRAM

On behalf of Dow AgroSciences LLC, I am please to submit the robust summaries in IUCLID format for 2,4-dichlorophenol sodium salt (Cas No.: 3757-76-4). As requested, the test plan has been posted onto the U.S. HPV Chemical Tracking System. All documents are in Adobe Acrobat (pdf) files.

We understand this information will be posted on the Internet for comments for a period of 120 days. Please forward comments to me at the following address:

Ms. Gail M. Garvin
Dow AgroSciences LLC
9330 Zionsville Road
Indianapolis, IN 46268

Sincerely,

Gail M. Garvin
Global Environmental, Health & Safety Specialist
(317) 337-3609

HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For

2,4-DICHLOROPHENOL, SODIUM SALT

Prepared by:

The Dow Chemical Company

May 22, 2003

PLAIN ENGLISH SUMMARY

This test plan addresses 2,4-dichlorophenol, sodium salt (CAS No. 3757-76-4). Existing data are summarized. No additional data will be collected under the HPV Challenge Program.

EXECUTIVE SUMMARY

The Dow Chemical Company hereby submits for review and public comment the test plan for 2,4-dichlorophenol, sodium salt, under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of The Dow Chemical Company to use new information in conjunction with a variety of existing data and scientific judgment/analyses to adequately characterize the SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this chemical.

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TEST PLAN FOR 2,4-DICHLOROPHENOL, SODIUM SALT

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TEST PLAN FOR 2,4-DICHLOROPHENOL, SODIUM SALT

I. INTRODUCTION

The Dow Chemical Company has committed voluntarily to develop screening level human health effects, environmental effects and fate, and physicochemical test data for 2,4-dichlorophenol, sodium salt under the Environmental Protection Agency's (EPA's) High Production Volume (HPV) Challenge Program (Program).

This plan identifies the chemical and its CAS number, identifies existing data of adequate quality for the chemical, and outlines testing planned to develop screening level data for the chemical under the Program. The objective of this effort is to identify and develop sufficient test data and/or other information to adequately characterize the human health and environmental fate for the chemical in compliance with the EPA HPV Program. Physicochemical data that are requested in this program will be provided.

II. DESCRIPTION OF 2,4-DICHLOROPHENOL, SODIUM SALT

A. The Chemical

2,4-dichlorophenol, sodium salt (CAS No. 3757-76-4) is used in the production of pesticides. This material has been studied to provide safe handling information.

III. TEST PLAN RATIONALE

A. Classification of the Chemical as a Production Chemical

1. Requirements

Classification of 2,4-dichlorophenol, sodium salt is as a production chemical under the EPA HPV program.

2. Toxicological Equivalency of 2,4-Dichlorophenol and the Sodium Salt of 2,4-Dichlorophenol

The OECD "Guidance for the Use of Structure-Activity Relationships (SAR) in the HPV Chemicals Programme" includes the opportunity to use SAR for health endpoints. The goal is to find toxicity data for an analog that can be used to address the testing needs of an HPV chemical and thus, reduce testing.

Valid analogs should have close structural similarity. Examples in the guidance document of surrogate data to characterize individual chemicals are as follows:

1) ***"Chemicals that are essentially the same in vivo. For example, different salts of the same anion or cation. The salts must fully dissociate in vivo and the counter ion must not contribute any more (or less) toxicity.***

2) *A chemical that metabolises to one (or more) compounds that have been tested. The metabolism must be rapid and complete."*

3) *Chemicals that have only minor structural differences that are not expected to have an impact on toxicity. All functional groups must be the same."*

Appendix B of the OECD "Guidance for the Use of Structure-Activity Relationships (SAR) in the HPV Chemicals Programme" provides examples from OECD SIDS cases and includes a specific example of acid-salt pairs (chloroacetic acid/sodium salt). In the case of the acid-salt pairs, no testing was considered necessary because the combined data for the acid/salt pair covered all of the SIDS endpoints. Similar to the SIDS approach for chloroacetic acid/sodium salt, the potential health effects of Na-DCP are adequately represented by the toxicological data for DCP based on the following physical-chemical data and SAR.

Although there does not appear to be any specific mammalian toxicological data available for the sodium salt of 2,4-dichlorophenol (Na-DCP), one would expect that Na-DCP would be toxicologically equivalent to 2,4-dichlorophenol (DCP) on a molar basis. The water solubility of DCP is 4 g/L at (25 degrees C) and the water solubility for Na-DCP is 7.05 g/L (20 degrees C, pH 7). The dissociation constant (pKa) for Na-DCP is 7.8, which is the same as DCP. Thus, Na-DCP would be expected to quickly dissociate to sodium and DCP in an aqueous environment such as the mammalian body. Upon the dissociation of Na-DCP, sodium would not be a significant factor in the metabolism or toxicity of DCP and thus, the systemic toxicity of Na-DCP would be equivalent to DCP on a molar basis. Therefore, the mammalian toxicological data for DCP are adequate for the evaluation of the potential hazards of the sodium salt of DCP.

Strong support for the predicted toxicological equivalency of DCP and Na-DCP is demonstrated in the extensive toxicological data base of the closely related molecule 2,4-dichlorophenoxyacetic acid (2,4-D) and its salts and esters. Numerous regulatory studies have been conducted with 2,4-D acid as well as the diethanolamine, dimethylamine, isopropylamine and triisopropanolamine salts and the butoxyethylhexyl and 2-ethylhexyl esters (Munro *et al.*, 1992; Kennepohl and Munro, 2001). A very extensive and complete toxicological database is available for 2,4-D acid. Toxicological studies with the amines and esters include pharmacokinetic, acute, subchronic dietary, 21-day dermal, developmental and genetic toxicity studies.

A joint meeting of the FAO Panel of Experts on Pesticide Residues and the WHO Expert Group on

Pesticide Residues (JMPR) has reviewed the extensive toxicological data for 2,4-D and its salts and esters (JMPR, 1997). These experts concluded "…that the toxicities of the salts and esters of 2,4-D were comparable to that of the acid." The basis for this conclusion is detailed in the following information abstracted from the Meeting's report:

"Pharmacokinetic studies with salts and esters of 2,4-D have shown that the salts dissociate and the esters are rapidly hydrolysed to 2,4-D. The similarity in the fate of 2,4-D and its salts and esters explains their similar toxicities.

"After dermal applications of 2,4-D to volunteers, 5.8% of the dose was absorbed within 120 h. When the acid and its dimethylamine (DMA) salt were applied, 4.5% of the acid and 1.8% of the salt were absorbed, and of this 85% of the acid and 77% of the salt were recovered in the urine 96 h after application.

"In six studies of toxicity rats fed diets containing the diethanolamine (DEA), [dimethylamine] DMA, isopropylamine (IPA), or tri-isopropanolamine (TIPA) salt or the butoxyethylhexyl (BEH) or 2-ethylhexyl (EH) ester at acid-equivalent doses of 0, 1, 15, 100, or 300 mg/kg bw per day for 13 weeks, the results demonstrated the comparable toxicity of the acid, salts and esters. The NOAEL was 15 mg acid equivalent per kg bw per day for all six compounds.

"Dogs were given gelatin capsules containing 2,4-D at 0, 0.3, 1, 3, or 10 mg/kg bw per day or diets containing 2,4-D, the DMA salt, or the EH ester at acid-equivalent doses of 0, 0.5, 1, 3.8, or 7.5 mg/kg bw per day for 13 weeks. Treatment-related findings were observed in the three studies at 3 mg/kg bw per day and above. The NOAEL was 1 mg acid equivalent per kg bw per day in all three studies.

"The developmental toxicity of the DEA, DMA, IPA, and TIPA salts and the BEH and EH esters was evaluated in pregnant rats after oral administration during days 6-15 of gestation. The acid-equivalent doses were 11, 55, or 110 mg/kg bw per day for the DEA salt; 12, 50, or 100 mg/kg bw per day for the DMA salt; 9, 25, 0r 74 mg/kg bw per day for the IPA salt; 12, 37, or 120 mg/kg bw per day for the TIPA salt; 17, 50, or 120 mg/kg bw per day for the BEH ester; and 10, 30, or 90 mg/kg bw per day for the EH ester. The maternal and developmental toxicities of the salts and esters of 2,4-D were comparable to those of the acid…The overall NOAELs were approximately 10 mg acid equivalent per kg bw per day for maternal toxicity and 50 mg acid equivalent per kg bw per day for developmental toxicity. [Developmental toxicity studies in pregnant rabbits with the same compounds resulted in similar findings.]

"In order to evaluate the dermal toxicity of 2,4-D and its salts and esters, rabbits received 15 dermal applications of the acid, the DEA, DMA, IPA, or TIPA salt or the BEH or EH ester at acid-equivalent doses of 0, 10, 100, or 1000 mg/kg bw per day for 6 h per day on

five days per week for 21 days. No systemic toxicity was observed at any dose, and no dermal toxicity [dermal lesion] was observed with the acid, the TIPA salt, or the BEH ester. Dermal lesions were observed in rabbits treated with the DEA, DMA, or IPA salt, or the EH ester at 100 mg/kg bw per day and above. The [dermal] lesions were characterized as acanthosis, hyperkeratosis, oedma, inflammation, and epidermal hyperplasia. The NOAEL was 10 mg acid equivalent per kg bw per day for dermal toxicity and 1000 mg acid equivalent per kg bw per day (the highest dose tested) for systemic toxicity."

The single-dose oral LD_{50} values for 2,4-D acid, esters (isooctyl, isobutyl, butoxyethanol and butyl), and salts (dimethylamine and sodium) ranged from 553 mg/kg (isobutyl ester in female rats) to 1090 mg/kg (dimethylamine salt in male rats) (Gorzinski *et al*., 1987). The LD_{50} values for the acid, esters, or salts, when expressed as acid equivalents, were consistent which suggests that the acute oral toxicity was due to 2,4-D per se. The acute dermal LD_{50} values in rabbits for 2,4-D acid, esters, and salts also were similar in that they generally were greater than 2000 mg/kg.

The acute dermal LD_{50} for DCP is 780 mg/kg bw in Sprague-Dawley rats. This value is based on a study that utilized test substance that was melted at 40° C in order to obtain the liquid form of the test material and more closely mimic accidental exposures. The potential for systemic toxicity or lethality from dermal exposure obviously is dependent upon a combination of the dermal absorption potential of a compound as well as its inherit systemic toxicity. Since DCP and dissociated Na-DCP would be expected to have equivalent systemic toxicity on a molar basis, differences in the systemic toxicity from dermal exposure of these compounds would be determined primarily by differences in dermal penetration.

Na-DCP has significantly less potential for systemic toxicity due to dermal exposure than DCP based on a comparison of physical-chemical properties as well as quantitative structure-permeability relationships (QSPRs) for percutaneous absorption. The partition coefficient (K_{ow}) for DCP is in the range of 2.92-3.25 (3.1 used for subsequent calculations) while the partition coefficient for Na-DCP is estimated at 0.12 (a lower K_{ow} would be expected for a salt which has higher water solubility). Molecular size (molecular weight) and hydrophobicity (as the logarithm of the octanol-water partition coefficient; Log K_{ow}) are the primary determinants of transdermal penetration (Moss *et al.*, 2002). Hydrophilic compounds have low skin permeability and hydrophobic compounds have high skin permeability; different Log K_{ow}-dependent QSARs can be used to predict skin permeability. High molecular weight compounds (>150 Dalton) with Log K_{ow} <0.5, such as Na-DCP, are in a category with the lowest permeability coefficient (K_p). On the other hand, high molecular weight compounds with 0.5 Log K_{ow} 3.5, such as DCP, have larger K_p values. Calculation of K_p values according to the equation of Cronin *et al*. (1999) [Log K_p = 0.77 log K_{ow} - 0.0103 MW - 2.33] results in a K_p ratio >300 for DCP:Na-DCP. QSPR analysis demonstrates that Na-DCP has significantly less potential for dermal absorption than DCP and thus, less potential for acute dermal toxicity than DCP.

The physical chemical properties of Na-DCP and DCP not only are the basis for expected differences in potential dermal toxicity, these properties also appear to be important in the recommendations for

immediate decontamination after dermal exposure. Reports of worker fatality cases from exposure to relatively small amounts of molten DCP prompted the U.S. Government to issue an advisory and notice of potential risk (EPA OPPT and OSHA, 2000). The advisory refers to research that indicates that octanol-water partition coefficients are indicative of lipophilicity which often correlates strongly with toxicity and skin penetration (Lopez *et al*., 1998). The researchers studied two homologous series, phenyl alcohols and p-alkylanilines, and found that the optimal lipohilicity for skin penetration, expressed as log P (n-octanol), was 3.1 which is very similar to the value for DCP. The advisory suggests that flushing skin exposed to DCP with an alkaline solution (soap, sodium bicarbonate, sodium carbonate, etc.) would convert the DCP to its ionized (salt) form, which would be more rapidly dissolved. The advisory goes on to state that a secondary benefit of an alkaline solution is that the ionized form of DCP would be much less lipophilic and, therefore, less readily absorbed into the skin. Thus, these recommendations are consistent with the conclusion of our QSPR analysis that indicated Na-DCP would have much less potential for dermal penetration and toxicity than DCP.

As prescribed by the OECD "Guidance for the Use of Structure-Activity Relationships (SAR) in the HPV Chemicals Programme," the above evaluation of the physical-chemical data and SAR indicate that the potential health effects of Na-DCP are adequately represented by the toxicological data for DCP. Utilization of the same classification, labeling and handling precautions for Na-DCP as for DCP would be conservative and clearly protective for human health even though no specific data are available for Na-DCP.

B. Human Health Effects

There are six mammalian toxicity endpoints in the HPV Program:

- Acute Toxicity
- Repeated Dose Toxicity
- Genetic Toxicity *In Vitro*
- Genetic Toxicity *In Vivo*
- Reproductive Toxicity
- Developmental Toxicity

Published and unpublished data for 2,4-dichlorophenol, as detailed in the attached Robust Summaries, satisfy the requirements of all required mammalian testing. We propose that no further testing is necessary. The attached Robust Summaries with the proposed testing provide adequate data to characterize the human health effects endpoints under the Program.

C. Ecotoxicity

There are three aquatic toxicity endpoints in the HPV Program:

- Acute Toxicity to Fish
- Acute Toxicity to Aquatic Invertebrates
- Toxicity to Algae (Growth Inhibition)

EPA identifies the following test methods to determine these endpoints: OECD Guideline 203, *Fish Acute Toxicity Test*; Guideline 202, *Daphnia sp., Acute Immobilization Test*; and Guideline 201, *Alga Growth Inhibition Test* [2] or equivalent studies.

Published and unpublished data for 2,4-dichlorophenol and its sodium salt, as detailed in the attached Robust Summaries, satisfies requirements for ecotoxicity data.

The existing data, along with the proposed testing, will be adequate to characterize ecotoxicity endpoints under the Program.

D. Environmental Fate

Predictive models as well as laboratory assays were used to develop meaningful data for 2,4-dichlorophenol. The environmental fate data include:

- Photodegradation
- Stability in Water (Hydrolysis)
- Transport and Distribution (Fugacity)
- Biodegradation

1. Photodegradation

Photodegradation was measured in laboratory testing, as detailed in the attached Robust Summaries.

2. Stability in Water (Hydrolysis Modeling)

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters [3]. Stability in water was measured experimentally, as detailed in the attached Robust Summaries.

3. Chemical Transport and Distribution In The Environment (Fugacity Modeling)

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model [6]. EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data*, which was prepared as guidance for the HPV Program.

In its document, EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent partitioned to 6 compartments within a unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. This model will be used to calculate distribution values for 2,4-dichlorophenol. A computer model, EPIWIN - version 3.02, will be used to calculate the properties needed to run the Level I EQC model.

4. Biodegradation Testing

Biodegradation is the utilization of a chemical by microorganisms as a source of energy and carbon. The parent chemical is broken down to simpler, smaller chemicals, which are ultimately converted to an inorganic form such as carbon dioxide, nitrate, sulfate, and water. Assessing the biodegradability of organic chemicals using a standard testing guideline can provide useful information for evaluating chemical hazard.

Biodegradation values for 2,4-dichlorophenol, sodium salt, as detailed in the attached Robust Summaries, were experimentally determined.

E. Physicochemical Properties

The physicochemical properties include:

- Melting Point
- Boiling Point
- Water solubility
- Octanol/Water Partition Coefficient

Data for physicochemical properties are summarized and detailed in the attached Robust Summaries.

IV. TEST PLAN SUMMARY

The following testing, modeling, and technical discussions will be developed for 2,4-dichlorophenol and thus for 2,4-dichlorophenol, sodium salt:

- Calculate fugacity data.

Summaries of results will be developed once the data are available. This test plan is expected to provide adequate data to characterize the human health effects and environmental fate and effects endpoints under the Program.

For reasons indicated in the above paragraphs, we do not believe additional data needs to be generated beyond the studies listed. Due to the nature of the chemical; the manner in which the chemical is manufactured, distributed, processed and used, the product stewardship measures taken to prevent exposure; and existing human/environmental data, we believe that our workers, the public and the environment are well protected from exposure to the material.

REFERENCES

Cronin, M.T.D., Dearden, J.C., Moss, G.P., and Murray-Dickson, G. (1999). Investigation of the mechanism of flux across human skin *in vitro* by quantitative structure-permeability relationships. European J. Pharm. Sci. 7: 325-330. [Cited by Moss *et al*., 2002]

Gorzinski, S.J., Kociba, R.J., Campbell, R.A., Smith, F.A., Nolan, R.J., and Eisenbrandt, D.L. (1987). Acute, Pharmacokinetic, and Subchronic Toxicological Studies of 2,4-Dichlorophenoxyacetic Acid. Fund. Appl. Toxicol. 9: 423-435.

Kennepohl, E. and Munro, I.C. (2001). Phenoxy Herbicides (2,4-D). In: Krieger, R. (Ed.), *Handbook of Pesticide Toxicology, Vol. 2, Agents*, Second Edition, Academic Press, San Diego, pp. 1623-1638.

Lopez, A., Faus, V., Diez-Sales, O., and Herraez, M. (1998). Skin permeation model of phenyl alcohols: comparison of experimental conditions. Internat. J. pharm. 173: 183-191.

Moss, G.P., Dearden, J.C., Patel, H., and Cronin, M.T.D. (2002). Quantitative Structure-Permeability Relationships (QSPRs) for Percutaneous Absorption. Toxicol. *In Vitro* 16: 299-317.

Munro, I.C., Carlo, G.L., Orr, J.C., Sund, K.G., Wilson, R.M., Kennepohl, E., Lynch, B.S., Jablinske,

M. and Lee, N.L. (1992). A Comprehensive, Integrated Review and Evaluation of the Scientific Evidence Relating to the Safety of the Herbicide 2,4-D. J. Am. Coll. Toxicol. 11: 559-664.

World Health Organization (WHO) (1997). Pesticide Residues in Food - 1996. Report of the Joint Meeting of the FAO Panel of Experts on Pesticide Residues in Food and the Environment and the WHO Expert Group on Pesticide Residues, Rome, Italy, September, 1996. FAO Plant Production and Protection Paper 140. Food and Agriculture Organization of the United Nations, pp. 31-38.

EPA Office of Pollution Prevention and Toxics and the Occupational Safety and Health Administration (EPA OPPT and OSHA) (February 15, 2000. Chemical Advisory and Notice of Potential Risk: Skin exposure to molten 2,4-Dichlorophenol (2,4-DCP) can cause rapid death.

EPIWIN. 1999. Estimation Program Interface for Windows, version 3.02. Syracuse Research Corporation, Syracuse, NY, USA.

201-15693

IUCLID

Data Set

Existing Chemical	:	ID: 3757-76-4
CAS No.	:	3757-76-4
Generic name	:	2,4-Dichlorophenol sodium salt

Producer Related Part

Company	:	The Dow Chemical Company
Creation date	:	24.01.2002

Substance Related Part

Company	:	The Dow Chemical Company
Creation date	:	24.01.2002
Memo	:	
Printing date	:	25.01.2002
Revision date	:	
Date of last Update	:	25.01.2002
Number of Pages	:	4
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	???

1.0.1 OECD AND COMPANY INFORMATION

Type	:	cooperating company
Name	:	The Dow Chemical Company
Partner	:	
Date	:	
Street	:	2020 Dow Center
Town	:	48674 Midland, Michigan
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

25.01.2002

1.0.2 LOCATION OF PRODUCTION SITE

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

1.3 IMPURITIES

1.4 ADDITIVES

1.5 QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.7 USE PATTERN

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.9 SOURCE OF EXPOSURE

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST. HARMLESS

1.13 STATEMENTS CONCERNING WASTE

1.14.1 WATER POLLUTION

1.14.2 MAJOR ACCIDENT HAZARDS

1.14.3 AIR POLLUTION

1.15 ADDITIONAL REMARKS

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Decomposition : yes at = 305 ° C
Sublimation :
Method : OECD Guide-line 102 "Melting Point/Melting Range"
Year : 2002
GLP : yes
Test substance : other TS
Test substance : 99.9% purity
Reliability : (1) valid without restriction
25.01.2002 (1)

2.2 BOILING POINT

Decomposition : yes
Method : OECD Guide-line 103 "Boiling Point/boiling Range"
Year : 2002
GLP : yes
Test substance : other TS
Test substance : 99.9% Purity
Reliability : (1) valid without restriction
25.01.2002 (2)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : < .0000000002 hPa at 20° C
Decomposition : no
Method other (calculated)
Year : 2002
GLP : yes
Test substance : other TS
Decomposition : no
Test substance : 99.9% purity
Reliability : (1) valid without restriction
25.01.2002 (2)

2.5 PARTITION COEFFICIENT

Log pow : = .12 at 20° C
Method other (calculated)
Year : 2002
GLP : yes
Test substance : other TS
Test substance : 99.9% purity
Reliability : (1) valid without restriction
25.01.2002 (1)

2.6.1 WATER SOLUBILITY

Value	:	= 6.04 g/l at 20 ° C
Qualitative	:	of high solubility
Pka	:	7.8 at 25 ° C
PH	:	= 4 at and ° C
Method	:	OECD Guide-line 105 "Water Solubility"
Year	:	2002
GLP	:	yes
Test substance	:	other TS
Remark	:	pKa is same as noted for 2,4-dichlorophenol.
Result	:	Water Solubility (at 20 C) pH 4= 6.04 g/L pH 7= 7.05 g/L pH 10= 142 g/L Unbuffered > 500 g/L As evident by the high water solubility in unbuffered water (>500 g/L) and as expected for a salt (by definition), the test substance completely dissociates in water. Therefore, the acid dissociation constant (pKa) for sodium salt of 2,4-dichlorophenol is the same as for 2,4-dichlorophenol.
Test substance	:	99.9% purity
Reliability	:	(1) valid without restriction

25.01.2002 (1)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Remark : 2,4-Dichlorophenol (2,4DCP) exhibits acute aquatic toxicity (LC50's in fish and EC50's in algae and Daphnia) between 1 and 10 mg/L. The sodium salt of 2,4DCP (2,4DCP-Na) will exhibit essentially equivalent toxicity values because the aquatic chemistry of these two chemical forms are essentially equivalent. First, the solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations encountered in the aquatic toxicity tests conducted on 2,4DCP (<100 mg/L). Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in aquatic testing facilities (pH = 7 to 8.5 at total alkalinities of 50 to 100 mg/L CaCO3), the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. To confirm this, the dissociation of 2,4-DCP and 2,4-DCP-Na and the effect of this dissociation on equilibrium pH was modeled using the USEPA computer program, MINTEQA2 version 3, a geochemical equilibrium and speciation model (Allison et al. 1991). An aqueous solution consisting of 50 mg/L CaCO3 in equilibrium with the atmosphere (pCO2=3x10-4 atm) was modeled containing 0, 10 and 100 mg/L 2,4-DCP and 0, 10 and 100 mg/L 2,4-DCP-Na (Appendix 1). In the absence of 2,4-DCP or 2,4-DCP-Na, MINTEQA2 calculated the equilibrium pH to be 8.27, consistent with the pH buffering ability of carbonate alkalinity in water (Stumm and Morgan, 1981; p. 183). MINTEQA2 calculated that addition of 10 mg/L or 100 mg/L 2,4-DCP would result in a very minimal pH change (pH=8.315, pH=8.339, respectively) and nearly identical aqueous speciation (74% phenoxide anion; 75% phenoxide anion, respectively). Addition of 10 mg/L or 100 mg/L 2,4-DCP-Na results in equivalent equilibrium pH (pH=8.336, pH=8.337, respectively) and equivalent aqueous speciation (both yield 75% phenoxide anion). Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, aquatic toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.

Reliability : (1) valid without restriction
25.01.2002 (3) (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Method :
Year : 2002
GLP :
Test substance :
Remark : 2,4-Dichlorophenol (2,4DCP) exhibits acute aquatic toxicity (LC50's in fish and EC50's in algae and Daphnia) between 1 and 10 mg/L. The sodium salt of 2,4DCP (2,4DCP-Na) will exhibit essentially equivalent toxicity values because the aquatic chemistry of these two chemical forms are essentially equivalent. First, the solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations encountered in the aquatic toxicity tests conducted on 2,4DCP (<100 mg/L). Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to

range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in aquatic testing facilities (pH = 7 to 8.5 at total alkalinities of 50 to 100 mg/L CaCO3), the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. To confirm this, the dissociation of 2,4-DCP and 2,4-DCP-Na and the effect of this dissociation on equilibrium pH was modeled using the USEPA computer program, MINTEQA2 version 3, a geochemical equilibrium and speciation model (Allison et al. 1991). An aqueous solution consisting of 50 mg/L CaCO3 in equilibrium with the atmosphere (pCO2=3x10-4 atm) was modeled containing 0, 10 and 100 mg/L 2,4-DCP and 0, 10 and 100 mg/L 2,4-DCP-Na (Appendix 1). In the absence of 2,4-DCP or 2,4-DCP-Na, MINTEQA2 calculated the equilibrium pH to be 8.27, consistent with the pH buffering ability of carbonate alkalinity in water (Stumm and Morgan, 1981; p. 183). MINTEQA2 calculated that addition of 10 mg/L or 100 mg/L 2,4-DCP would result in a very minimal pH change (pH=8.315, pH=8.339, respectively) and nearly identical aqueous speciation (74% phenoxide anion; 75% phenoxide anion, respectively). Addition of 10 mg/L or 100 mg/L 2,4-DCP-Na results in equivalent equilibrium pH (pH=8.336, pH=8.337, respectively) and equivalent aqueous speciation (both yield 75% phenoxide anion). Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, aquatic toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.

Reliability : (1) valid without restriction
25.01.2002 (3) (4)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Method :
Year : 2002
GLP :
Test substance :
Remark : 2,4-Dichlorophenol (2,4DCP) exhibits acute aquatic toxicity (LC50's in fish and EC50's in algae and Daphnia) between 1 and 10 mg/L. The sodium salt of 2,4DCP (2,4DCP-Na) will exhibit essentially equivalent toxicity values because the aquatic chemistry of these two chemical forms are essentially equivalent. First, the solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations encountered in the aquatic toxicity tests conducted on 2,4DCP (<100 mg/L). Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in aquatic testing facilities (pH = 7 to 8.5 at total alkalinities of 50 to 100 mg/L CaCO3), the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. To confirm this, the dissociation of 2,4-DCP and 2,4-DCP-Na and the effect of this dissociation on equilibrium pH was modeled using the USEPA computer program, MINTEQA2 version 3, a geochemical equilibrium and speciation model (Allison et al. 1991). An aqueous solution consisting of 50 mg/L CaCO3 in equilibrium with the atmosphere (pCO2=3x10-4 atm) was modeled containing 0, 10 and 100 mg/L 2,4-DCP and 0, 10 and 100 mg/L 2,4-DCP-Na (Appendix 1). In the absence of 2,4-DCP or 2,4-DCP-Na, MINTEQA2 calculated the equilibrium pH to be 8.27, consistent with the pH buffering ability of carbonate alkalinity in water

(Stumm and Morgan, 1981; p. 183). MINTEQA2 calculated that addition of 10 mg/L or 100 mg/L 2,4-DCP would result in a very minimal pH change (pH=8.315, pH=8.339, respectively) and nearly identical aqueous speciation (74% phenoxide anion; 75% phenoxide anion, respectively). Addition of 10 mg/L or 100 mg/L 2,4-DCP-Na results in equivalent equilibrium pH (pH=8.336, pH=8.337, respectively) and equivalent aqueous speciation (both yield 75% phenoxide anion). Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, aquatic toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.

Reliability : (1) valid without restriction
25.01.2002 (3) (4)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VITRO‘

5.7 CARCINOGENITY

5.8 TOXICITY TO REPRODUCTION

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.10 OTHER RELEVANT INFORMATION

5.11 EXPERIENCE WITH HUMAN EXPOSURE

(1) Unpublished data, Dow Agrosciences LLC.

(2) Unpublished data, Dow Agrosciences LLC

(3) Allison, J.D., D.S. Brown and K.S. Novo-Gradac. 1991. MINTEQA2/PRODEFA2: A Geochemical Assessment Model for Environmental Systems. EPA/600/3-91/021. Assessment Branch, Environmental Research Laboratory, Athens, GA, USA.

(4) Stumm, W. and J.J. Morgan. 1981. Aquatic Chemistry: An Introduction Emphasizing Chemical Equilibria in Natural Waters, 2nd Edition. John Wiley and Sons, Inc. New York. p. 183.

7.1 END POINT SUMMARY

Chapter : 4
Remark : 2,4-Dichlorophenol (2,4DCP) exhibits acute aquatic toxicity (LC50's in fish and EC50's in algae and Daphnia) between 1 and 10 mg/L. The sodium salt of 2,4DCP (2,4DCP-Na) will exhibit essentially equivalent toxicity values because the aquatic chemistry of these two chemical forms are essentially equivalent. First, the solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations encountered in the aquatic toxicity tests conducted on 2,4DCP (<100 mg/L). Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in aquatic testing facilities (pH = 7 to 8.5 at total alkalinities of 50 to 100 mg/L CaCO3), the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. To confirm this, the dissociation of 2,4-DCP and 2,4-DCP-Na and the effect of this dissociation on equilibrium pH was modeled using the USEPA computer program, MINTEQA2 version 3, a geochemical equilibrium and speciation model (Allison et al. 1991). An aqueous solution consisting of 50 mg/L CaCO3 in equilibrium with the atmosphere (pCO2=3x10-4 atm) was modeled containing 0, 10 and 100 mg/L 2,4-DCP and 0, 10 and 100 mg/L 2,4-DCP-Na (Appendix 1). In the absence of 2,4-DCP or 2,4-DCP-Na, MINTEQA2 calculated the equilibrium pH to be 8.27, consistent with the pH buffering ability of carbonate alkalinity in water (Stumm and Morgan, 1981; p. 183). MINTEQA2 calculated that addition of 10 mg/L or 100 mg/L 2,4-DCP would result in a very minimal pH change (pH=8.315, pH=8.339, respectively) and nearly identical aqueous speciation (74% phenoxide anion; 75% phenoxide anion, respectively). Addition of 10 mg/L or 100 mg/L 2,4-DCP-Na results in equivalent equilibrium pH (pH=8.336, pH=8.337, respectively) and equivalent aqueous speciation (both yield 75% phenoxide anion). Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, aquatic toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.
Reliability : (1) valid without restriction
25.01.2002

Chapter : 5
Remark : The solubility of 2,4DCP (4000 mg/L; 25 mM) and 2,4DCP-Na (7050 mg/L; 38 mM) indicate that both forms are freely soluble at the concentrations likely to be encountered in mammalian testing. Both chemical forms exhibit high solubility because they readily dissociate in aqueous solution. The aqueous dissociation constant (pKa) for 2,4-DCP has been reported to range from 7.6 to 7.89, suggesting that at pH values likely to be encountered in the mammalian intestinal tract, the majority of the 2,4-DCP is likely to be in the anionic (phenoxide) form. Furthermore, this speciation is not significantly affected by the starting form of the test material (sodium salt of phenol) because these forms readily dissociate in solution to yield the phenoxide anion. Thus, regardless of whether that sodium salt of 2,4-DCP or the phenol form of 2,4-DCP are added to aqueous solutions, the same speciation occurs in solution. Therefore, mammalian toxicity testing of the sodium salt of 2,4-DCP would yield results equivalent to that already achieved in the testing of 2,4-DCP.
Reliability : (1) valid without restriction

25.01.2002

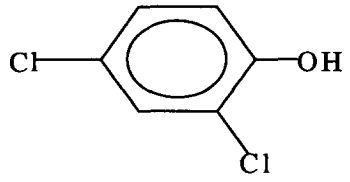
7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

SIAM 15, 22-25 October 2002

FR/ICCA

SIDS INITIAL ASSESSMENT PROFILE

CAS No.	120-83-2
Chemical Name	2,4-Dichlorophenol
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR

Human Health

Free 2,4-dichlorophenol (2,4-DCP) does not accumulate in tissues. 2,4-DCP is a strong uncoupler for oxidative phosphorylation. It is rapidly metabolised into its glucuronate conjugate, its major metabolite, and is mainly excreted in this form via urine.
The acute oral toxicity is low: LD50 1276-1352 mg/kg b.w. when tested in CD 1 mice. The dermal toxicity is moderate: LD_{50} in Sprague Dawley rats was 780 mg/kg with molten substance at 40°C. Further occupational deaths have been reported in five cases. Accidents generally occurred in the same way: workers died after being sprayed with molten (60°C) 2,4-dichlorophenol. US-EPA concludes that contact with only 1% of the body surface may lead to death. The skin irritation tests with 2,4-dichlorophenol reports the substance to be "corrosive" to skin and risk of serious damage to the eyes is expected.

The skin sensitisation potential has not been assessed. Its evaluation may be considered as unwanted due to the necessity to avoid contact with corrosive materials. Chloracnea appears at human exposure to a mixture of chlorophenols containing 2,4-dichlorophenol.

The 2-year study (Fischer 344 rat) was chosen to establish an overall NOAEL, after prolonged treatment with 2,4-dichlorophenol, of 440 mg/kg bw/d for male and above 250 mg/kg bw/d for female, which is in agreement with the findings in the other studies. In a 90 days repeated dose toxicity study dietary administration produced bone marrow degeneration at about 800 mg/kg bw/d in females or at 1500 mg/kg bw/d in males; at 3000 mg/kg bw/d these effects were not seen. The general appearance was affected at the top dose of 3000 mg/kg bw/d.

The genetic toxicity is assessed by *in vitro* and *in vivo* studies. *In vitro*, most of the test results were negative. An *in vivo* micronucleus test, an unscheduled DNA synthesis test and two sister chromatid exchange assays were all negative. It is concluded that the material is not genotoxic as the results of the *in vivo* tests are negative.

No evidence of carcinogenic activity was reported in rat and in mouse exposed orally for two years. These results are supported by the conclusion of the IARC: although polychlorophenols and their salts are classified in group 2B, there is evidence suggesting lack of carcinogenicity of 2,4-DCP in experimental animals (IARC, 1999).

In a one-generation study, no effect was observed via drinking water at 500 mg/kg bw/d in mice. A non-conventional one-generation study with rats using dose levels up to 15 mg/kg bw/d did not show any significant effect on reproduction parameters. The only significant effect was an increase of some hematologic parameters (red blood cell and hemoglobin), in the F1 generation at 15 mg/kg bw/d, observed after a 14 month exposure. *In vitro* studies showed no effect on penetration of sperm in mouse ova.

There were no teratogenic effects observed in rats exposed by gavage at doses up to 750 mg/kg bw/d. The NOAEL

for maternal effects is <200 mg/kg bw/d, (lowest dose tested) and the NOAEL for foetal effects is 375 mg/kg bw/d.

In these studies considering developmental toxicity and teratogenicity, 2,4-dichlorophenol has been reported to have toxic effects on foetuses at dose levels causing maternal effects (decrease in the litter size, delayed fetal development, increase in the organ weights).

The hormone disruption potency of 2,4-DCP was shown in only one *in vitro* test considered to be invalid. In another *in vitro* tests on estrogenic activity (competitive binding and response to proliferation culture) results were negative. Results were also negative in two *in vivo* tests (a uterotrophic assay and a Hershberger assay). A two generation reproductive study of 2,4-DCP is now underway in Japan (METI). By incorporating the results of this study into existing findings, the endocrine disruption effects of 2,4-DCP will be comprehensively assessed.

Environment

2,4-DCP is a white solid in crystal or needle forms. It has a low vapour pressure at room temperature (0.16 hPa at 25 °C). The water solubility of 2,4-DCP is 4.5 g/l at 25 °C, but since the pKa is 7.89, which falls in the pH range of environmental waters (approximately 6-9), the extent of dissociation of 2,4-DCP may vary significantly. The measured log Pow is 3.21-3.25 at 20°C.

Based on its vapour pressure, 2,4-DCP is expected to have a low volatility from dry soil surfaces. In contrast, photodegradation should be an important means of removing 2,4-DCP from clear surface water. Atmospheric oxidation half-life is estimated by QSAR to be 3.6 days. Hydrolysis is not expected to occur: halogenated aromatics and phenols are generally resistant to hydrolysis. Mechanisms other than photodegradation and microbial degradation, as adsorption by organic matter present within the sediments, catalysis at the surface of silica or oxidation, may also be involved in the disappearance of 2,4-DCP from water. Since the pKa is around 7.8, 2,4-DCP will exist in water and sediment in a partially dissociated state which may affect its transport and reactivity. Similarly in soil, the ionised form (in alkaline soil) is poorly adsorbed, whereas the neutral form (acid soil) is expected to undergo more adsorption. Adsorption will also increase with increasing organic matter content.

Biodegradation studies have shown that 2,4-DCP was not readily biodegradable, but it was inherently degradable only in the presence of adapted microflora, both in aerobic and anaerobic conditions. Anaerobic degradation of 2,4-DCP produced 4-chlorophenol as the major product. The BCFs of 7.1 to 69 in carp suggest that bioaccumulation in aquatic organisms is low.

Aquatic effects

In acute toxicity studies, the lowest LC_{50} values are 1.7 mg/L for freshwater fish and 1.4 mg/l for *Daphnia magna*. For aquatic plants, results on Lemna are available, leading to EC_{50} (7d) = 1.5 mg/L (endpoint: vegetative frond reproduction). In chronic toxicity studies, a NOEC of 0.29 mg/l for a fish, of 0.41 mg/L for Lemna (endpoint: vegetative frond reproduction) and a NOEC of 0.21 mg/l (endpoint: reproductivity rate) for *Daphnia magna* have been obtained. In a non-standard valid test on net spinning behaviour of the Trichoptera larvae, A LOEC value of 0.0035 mg/l was derived.

Despite the numerous consistent data available on fish, Daphnia and algae, issued from acute and chronic toxicity studies, due to the uncertainties on ecological relevance of the endpoint of the Trichoptera study, no final decision was made regarding PNEC derivation.

Tests with activated sludge resulted in EC50 values of 32 – 73 mg/l. Tests with *Pseudomonas putida* and *Tetrahymena pyriformis* resulted in EC50 values of 133 and 4.5 – 12.6 mg/l, respectively. Test with nitrifying bacteria resulted in a EC50 value of 0.15 mg/l. This latter value could be used for the derivation of a PNEC.

Terrestrial effects

The LC50 for earthworm is 125 mg/kg dw and for plants the EC50 is 316 mg/kg dw. The EC10 in a 34 day test with *Folsomia candida* was 0.7 mg/kg dw.

Exposure

The production volume of 2,4-dichlorophenol was 2000 to 5000 tonnes per year in France.

The use is non-dispersive, as an intermediate for synthesis in chemical industry. The product is not dispersed or transported outside of the site in the Sponsor country, the process functions in a closed system. The principle hazard for manufacturers or users can be burns by accidents at debottlenecking with a temperature higher than 60°C. In closed systems if there is a leak the penetrating odour of 2,4-dichlorophenol gives an alert.

The possible sources of 2,4-DCP in the environment are through the degradation of 2,4-D (2,4-dichlorophenoxy acetic acid, herbicide), or potentially chlorination of phenol-containing water.

RECOMMENDATION

The chemical is currently of low priority for further work.

RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

Human Health and Environment

The chemical possesses properties indicating a hazard for human health and the environment. Based on data presented by the Sponsor country, exposure to humans and the environment is anticipated to be low, and therefore this chemical is currently of low priority for further work in the SIDS Programme. Countries may desire to investigate any exposure scenarios that were not presented by the Sponsor country. The main source for 2,4-DCP measured in the environment appears to be through degradation of the pesticide 2,4-D.

In other programmes: a two generation study in rat is under-way to complete the assessment of its endocrine disrupter potential (METI, Japan) and for the environment, an EU evaluation (in relation to the Community Strategy for Endocrine Disrupters) is ongoing.